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Analytic model of harmonic generation in the low-gain FEL regime*

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Abstract

Harmonic generation using free electron lasers (FELs) requires two undulators: the first uses a seed laser to modulate the energy of the electron beam; the second undulator uses the subsequently bunched beam to radiate at a higher harmonic. These processes are currently evaluated using extensive calculations or simulation codes which can be slow to evaluate and difficult to set up. We describe a simple algorithm to predict the output of a harmonic generation beamline in the low-gain regime based on trial functions for the output radiation. Full three-dimensional effects are included. This method has been implemented as a Mathematica script which runs rapidly and can be generalized to include effects such as asymmetric beams and misalignments. This method is compared with simulation results using the FEL code GENESIS, both for single stages of harmonic generation and for the LUX project, a design concept for an ultrafast X-ray facility, where multiple stages upshift the input laser frequency by factors of up to 200.

INTRODUCTION

There is growing interest in using seeded electron beams to drive a free electron laser (FEL), rather than relying on amplification of noise. This allows for controlled timing and pulse structure. The seed can be a laser field which is then amplified by the FEL instability, or it can be an initial current variation (bunching) in the electron beam. The second method allows for harmonic generation, where the output wavelength can be at a harmonic of the initial perturbation [1]. The possible use of multiple stages of such harmonic generation is an area of active study, for example in the LUX [2] project, which is an R&D project in ultrafast X-ray production. Here, an analytic model for predicting and optimizing the FEL output from an idealized, pre-bunched electron beam is presented, with emphasis on harmonic generation. While previous examinations of seeded electron beams either assume the laser field structure in advance [3, 4], or rely on summations over single-particle radiation fields [5], this formalism uses a trial-function approach to obtain simple analytic prescriptions for determining the output laser field. These expressions only apply to FELs in the low-gain regime, but include the full 3-dimensional dynamics. A set of scripts implemented in Mathematica allows for rapid calculation of the dominant mode produced by a seeded electron beam, as well as a means to rapidly optimize FEL and beam parameters.

ANALYTIC MODEL

The output from the radiating undulator, or radiator, is here approximated as a simple Gaussian mode, but is otherwise kept arbitrary:

$$E_y = \Re E_0 e^{i\Phi_0} G(x, y, s) \exp(iks - i\omega t), \quad (1)$$

where

$$G(x, y, s) \equiv \frac{Z_R}{Z_R + i(s - s_0)} \exp \left[-\frac{1}{2} \frac{k(x^2 + y^2)}{Z_R + i(s - s_0)} \right] \quad (2)$$

characterizes the structure of the mode. The laser wavelength is $\lambda = 2\pi/k$, the frequency $\omega = ck$, and Z_R is the Rayleigh length. The longitudinal coordinate s represents the position along the undulator, and at $s = s_0$ the laser is at its waist with spot size $(Z_R/2k)^{1/2}$. It is possible to generalize this to include higher-order transverse modes. Note that this field only characterizes the output from the radiator, and so will be described by vacuum field solutions.

The particle motion due to the undulator is

$$v_u \simeq \frac{\sqrt{2}c}{\gamma} a_u \sin(k_u s), \quad (3)$$

where the undulator period is $\lambda_u = 2\pi/k_u$, the normalized field strength is $a_u = eB_0/mck_u$, and B_0 is the RMS dipole field on axis from the undulator. The dipole field on axis is taken to be $B_x = -\sqrt{2}B_0 \cos(k_u s)$. For a single particle, the forward motion satisfies

$$t = t(s=0) + \frac{s}{v_z} - \frac{a_u^2}{4ck_u\gamma^2} \sin(2k_u s), \quad (4)$$

where v_z is the average forward velocity, and the last term arises from the motion in a planar undulator.

The change in energy of a particle is given by

$$\begin{aligned} \frac{d\gamma}{ds} &= -\frac{e}{mc^2} \frac{E_y v_u}{v_z} \\ &\simeq -\Re k a_L G(x, y, s) e^{i(ks - \omega t)} \frac{\sqrt{2} a_u}{\gamma} \sin(k_u s), \end{aligned} \quad (5)$$

where the normalized (complex-valued) laser field is

$$a_L = \frac{eE_0}{mc^2 k} e^{i\Phi_0}. \quad (6)$$

Averaging over an undulator period yields

$$\frac{d\gamma}{ds} = -\Im \frac{\sqrt{2}k}{2\gamma} a_u a_L G(x, y, s) \mathbb{J}(\xi) e^{i\Psi}, \quad (7)$$

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where $\mathbb{J}(\xi) \equiv J_0(\xi) - J_1(\xi)$, $\xi \equiv ka_u^2/4k_u\gamma^2$, and the ponderomotive phase $\Psi \equiv ks - \omega t + k_u s$. To leading order in $1/\gamma^2$, this phase evolves according to

$$\frac{d\Psi}{ds} = k_u + k(1 - c/v_z) \simeq k_u - \frac{k}{2}(1/\gamma^2 + v_\perp^2/c^2), \quad (8)$$

where v_\perp^2 is also averaged over an undulator period.

The undulator field increases with strength off-axis. For an undulator with equal focusing in both planes, and taking into account the slight transverse dependence of a_u in Eq. (3), the average of v_\perp^2/c^2 over an undulator period is roughly given by

$$\frac{v_\perp^2}{c^2} = \frac{a_u^2}{\gamma^2} + \frac{2(J_x + J_y)}{\gamma\beta_u}, \quad (9)$$

where $\beta_u \equiv \sqrt{2}\gamma/a_u k_u$ is the matched beta function for the undulator, and J_x, J_y are the transverse actions for this value of the beta function:

$$J_x \equiv \frac{\gamma}{2} \left[\frac{x^2}{\beta_u} + \beta_u \left(\frac{dx}{ds} \right)^2 \right], \quad (10)$$

and similarly for J_y . If external focusing is used, however, then J_x and J_y will no longer be constants of the motion.

Now we can expand out the equation for Ψ ,

$$\frac{d\Psi}{ds} \simeq k_u \left[-\frac{\delta k}{k_r} + 2\frac{\gamma - \gamma_r}{\gamma_r} - \frac{2a_u\delta a_u}{1 + a_u^2} - \sqrt{2}\frac{a_u}{1 + a_u^2}k_u(J_x + J_y) \right], \quad (11)$$

where we define $k = k_r + \delta k$, and the resonant wave vector is

$$k_r \equiv \frac{2\gamma_r^2}{1 + a_u^2}k_u. \quad (12)$$

The detuning can be expressed equivalently in terms of δk or as a shift in undulator strength δa_u . Using the resonance condition, the argument of the Bessel functions in Eq. (7) is $\xi = (1/2)a_u^2/(1 + a_u^2)$.

Finally, there is the expression for the laser field, assuming the power given up by the electron beam goes into a single mode. For the mode defined by Eq. (2), the power is

$$P_L = \frac{1}{2}c\epsilon_0 E_0^2 \pi \frac{Z_R}{k} = \frac{1}{8}kZ_R \frac{mc^3}{r_e} |a_L|^2, \quad (13)$$

where $r_e = e^2/(4\pi\epsilon_0 mc^2)$. By conservation of energy, the change in power is given by $dP_L/ds = -(I/e)mc^2 \langle (d\gamma/ds) \rangle$, where I is the peak current and $\langle d\gamma/ds \rangle \equiv \int d\bar{X} f(\bar{X}) (d\gamma/ds)$. The term \bar{X} is used as a shorthand to represent the full set of 6D phase space variables, and the distribution function $f(\bar{X})$ is normalized so that $\int d\bar{X} f(\bar{X}) = 1$. Noting that P_L scales as $|a_L|^2$, we have

$$\frac{d|a_L|}{ds} = \frac{I}{I_A} \frac{2\sqrt{2}a_u}{\gamma Z_R} \mathbb{J}(\xi) \Im \langle e^{i\Phi_0} G(x, y, s) e^{i\Psi} \rangle, \quad (14)$$

where $I_A \equiv 4\pi\epsilon_0 mc^3/e \simeq 17$ kA. This is the electric field generated by the net bunching of the electron beam, and we wish to generalize this to include the possibility of having no seed pulse, but a pre-bunched beam. Using the relation that $d|a_L|/ds = \Re(e^{-i\Phi_0} da_L/ds)$, Eq. (14) can be generalized to

$$\frac{da_L}{ds} = i \frac{I}{I_A} \frac{2\sqrt{2}a_u}{\gamma Z_R} \mathbb{J}(\xi) \langle G^*(x, y, s) e^{-i\Psi} \rangle. \quad (15)$$

The above average is a correction to the usual bunching parameter, $b \equiv \langle \exp(-i\Psi) \rangle$. The generalized bunching parameter will be defined as

$$B(s) \equiv \langle G^*(x, y, s) e^{-i\Psi} \rangle. \quad (16)$$

Harmonic generation, for example in the LUX design concept, uses a seed laser to generate an energy modulation in one undulator, which is then converted into microbunching by means of a chicane. The additional slippage which results from the chicane is characterized by the parameter R_{56} , defined by $c\Delta t = R_{56}(\gamma - \gamma_0)/\gamma_0$. Following this, the bunched beam produces radiation while passing through a second undulator. Because the bunching includes Fourier components at harmonics of the initial laser seed, this second, radiating undulator can be tuned to a higher harmonic of the laser seed. Here, we consider a simplified case where the modulator applies an energy modulation which depends solely on the phase Ψ of the electrons. The energy distribution after modulation then takes the form

$$f(\bar{X}) \propto H[(\gamma - \gamma_0 - \kappa_x J_x - \kappa_y J_y + \gamma_M \sin \Psi)/\Delta_\gamma]. \quad (17)$$

We will consider both Gaussian and uniform energy profiles, where Δ_γ is equal to the RMS energy spread and maximum deviation, respectively. This energy distribution includes the possibility for “beam conditioning”, where there is a correlation between energy and transverse amplitude. The transverse component of the distribution function is $\exp(-J_x/\epsilon_x - J_y/\epsilon_y)$, where ϵ_x is the normalized emittance in the x -plane. The wave vector in the following radiator will be a harmonic, n , of the resonant wave vector in the modulator. Thus, we will want to look at the quantity $\exp(-in\Psi)$ instead of the bunching at the first harmonic.

After the modulator, the beam passes through a dispersive section with a resulting phase shift $\Delta\Psi = k_0 R_{56}(\gamma - \gamma_0)/\gamma_0$, where k_0 is the wave vector corresponding to the modulator. After this dispersive section, the higher harmonic bunching will be given by

$$|\langle e^{-in\Psi} \rangle| = J_n(kR_{56}\gamma_M/\gamma_0) F_\gamma(kR_{56}\Delta_\gamma/\gamma_0), \quad (18)$$

where $k = nk_0$ is the wave vector of the higher harmonic. The function F_γ depends on the form of the energy distribution:

$$F_\gamma(x) = \begin{cases} \exp(-x^2/2), & \text{Gaussian} \\ (\sin x)/x, & \text{uniform.} \end{cases} \quad (19)$$

The averages over particle energy and ponderomotive phase within the radiator yield the same F_γ and Bessel

function as above for the initial bunching parameter, but with kR_{56} replaced with $kR_{56} + 2k_us$. In addition to $G^*(x, y, s)$, there are extra phase terms which depend on transverse coordinates which must be considered. Below, we assume that the beam has the properly matched beta function for the undulator. The final result for the generalized bunching at the higher harmonic is

$$\begin{aligned}
B(s) = & \exp \left[ik_us \left(\frac{\delta k}{k_r} - 2 \frac{\gamma_0 - \gamma_r}{\gamma_r} \right) \right] \\
& \times J_n \left[(kR_{56} + 2k_us) \frac{\gamma_M}{\gamma_0} \right] \\
& \times F_\gamma \left[(kR_{56} + 2k_us) \frac{\Delta\gamma}{\gamma_0} \right] \frac{Z_R}{Z_R - i(s - s_0)} \\
& \times F_\epsilon(\epsilon_x, c_x(s), s) F_\epsilon(\epsilon_y, c_y(s), s), \quad (20)
\end{aligned}$$

where

$$\begin{aligned}
F_\epsilon(\epsilon, c, s) = & (1 - ic\epsilon)^{-1/2} \\
& \times \left(1 - ic\epsilon + \frac{k_r\beta_u\epsilon/\gamma_0}{Z_R - i(s - s_0)} \right)^{-1/2}. \quad (21)
\end{aligned}$$

The quantity

$$c_x(s) \equiv 2k_us \left(\frac{\sqrt{2}}{2} k_u \frac{a_u}{1 + a_u^2} - \frac{\kappa_x}{\gamma_r} \right) - \frac{\kappa_x}{\gamma_r} kR_{56} \quad (22)$$

is related to the slippage due to transverse emittance, and similarly for $c_y(s)$. If it is the strength of the undulator which is being tuned, the detuning term $\delta k/k_r$ can be replaced with $2a_u\delta a_u/(1 + a_u^2)$.

The laser field at the end of the radiator is then given by

$$a_L = i \frac{I}{I_A} \frac{2\sqrt{2}a_u}{\gamma Z_R} \text{JJ}(\xi) \int_0^L B(s) ds, \quad (23)$$

and the laser power is given by Eq. (13).

TRIAL FUNCTIONS

The result is still not fully defined because Z_R and s_0 are free parameters. In general, after fixing Z_R and s_0 , any radiation field can be described using a sum of normal modes, but here we are restricting attention to a single, Gaussian mode. Because the exact result will include the power contained within all these modes, the analytic result is expected to always fall below the correct value. This suggests varying the free parameters to maximize the output power, yielding a greatest lower bound to the correct result.

This method is essentially a trial function approach, and any trial function which is a valid vacuum laser field can be used. The closer the trial function is to the exact result, the more accurate this estimate for the power will be. Furthermore, the prediction for the laser power is expected to be second-order accurate compared to the optimized trial function; in other words, even a poor approximation to

the laser field can result in a good estimate for the output power. In the configurations being considered, a pure Gaussian mode is expected to be a reasonable approximation to the FEL output except in the emittance-dominated regime, $\epsilon/\gamma_0 \gtrsim \lambda/(4\pi)$. In this paper, only a simplified FEL configuration is considered, but the trial function method applies to more general cases as well.

The resulting integrals are simple enough to implement as a Mathematica script, which allows for rapid optimization. Because the optimization procedure is to maximize the output power, any additional constraints (undulator field, R_{56} , or energy modulation) can be simultaneously optimized to obtain the largest possible output power. Thus any optimizations performed on the beamline can occur simultaneously with the trial function optimization for Z_R and s_0 , greatly reducing the computational time required.

SIMULATION RESULTS

FEL simulations using the GENESIS code [6] have been compared with this analytic theory. Two cases are considered, the first stage of a cascade which converts 200 nm wavelength to 50 nm, and the final stage which converts 3.13 nm wavelength to 1.04 nm. All sections are assumed to use planar undulators.

For a given set of trial functions, the analytic model finds the closest fit to the actual radiation, and predicts a lower bound on the total output power. Even if the trial function does not accurately represent the radiation field produced by the FEL, the prediction for the output power may still serve as a good estimate.

Table 1: Comparison between analytic model and simulations using GENESIS for two case studies.

Case	Results	Analytic Theory	GENESIS:	
			$M^2 \equiv 1$	fit M^2
50 nm	P_L (MW)	130.3	134.2	134.2
	Z_R (m)	1.12	0.94	0.97
	s_0 (m)	1.20	1.19	1.21
	M^2	$\equiv 1$	$\equiv 1$	1.04
1.04 nm	P_L (MW)	35.1	39.0	39.0
	Z_R (m)	52.7	49.0	33.0
	s_0 (m)	-10.4	-14.6	0.73
	M^2	$\equiv 1$	$\equiv 1$	1.72

The electron beam parameters are: $I = 500$ A, $\gamma_0 = 6067$, and the normalized emittances are $\epsilon_x = \epsilon_y = 2 \mu\text{m}$. Results for the two cases considered are given in Table 1. The transverse mode structure of the output radiation is described in terms of the M^2 parameter, which is the ratio of the emittance of the laser to the minimum emittance, $\lambda/4\pi$. This parameter can also be described as the ratio of the idealized Rayleigh length for the given waist diameter to the observed Rayleigh length. In terms of power flux, the RMS width of the laser at the waist is $(\lambda M^2 Z_R/4\pi)^{1/2}$. For the first stage, producing radiation at 50 nm by going to

the fourth harmonic, the energy modulation is $\gamma_M = 2.68$, and the chicane is set to an optimized value of $R_{56} = 92 \mu\text{m}$. The radiating undulator has an 8 cm period and is 2.4 m long. The electron beam is taken to be matched to the undulator, with $\beta = 16.28$ m. The resonant undulator strength is $a_u = 6.709$, but optimal performance occurs at $a_u = 6.686$. An analysis of the GENESIS results show that 7.8 MW of power lies outside the predicted Gaussian mode. The analytic theory underestimates the total power by 3.9 MW, a relative error of 3%. For the final stage, producing radiation at 1.04 nm by going to the third harmonic, the energy modulation is $\gamma_M = 1.10$, and the idealized chicane uses $R_{56} = 3.2 \mu\text{m}$. The radiating undulator has a 2.8 cm period and is 8.4 m long. The electron beam is taken to be matched to the undulator, with $\beta = 29.00$ m. The resonant undulator strength is $a_u = 1.3186$, but optimal performance occurs at $a_u = 1.3181$. In the simulation results, 2.3 MW of power lies outside the predicted Gaussian mode. The analytic theory underestimates the total power by 3.9 MW, a relative error of 10%. A generalization to trial functions having two or more transverse modes would be desirable for more accurate results.

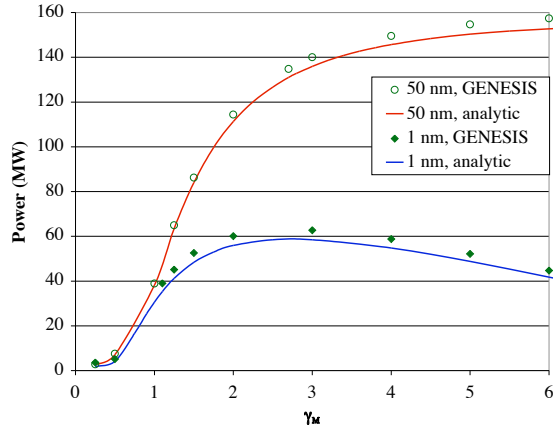


Figure 1: Comparison of analytic theory with simulations using GENESIS. Results for harmonic generation at 50 nm and 1.04 nm, as the energy modulation γ_M is varied.

The dependence of the output radiation on the energy modulation is shown in Figure 1, and also shows good agreement between the analytic model and numerical simulations. The value of R_{56} is re-optimized for each case. For short wavelengths, FEL performance is more sensitive to the energy spread, as slippage along the length of the undulator leads to debunching of the electron beam. The optimal power of 60 MW can only be increased either by using a different undulator design or by lowering the harmonic number.

The agreement between theory and simulations only falters for the 1.04 nm case, when the magnetic fields are tuned below the resonant value, as shown in Figure 2. Far from resonance, there is roughly 5 MW of power in

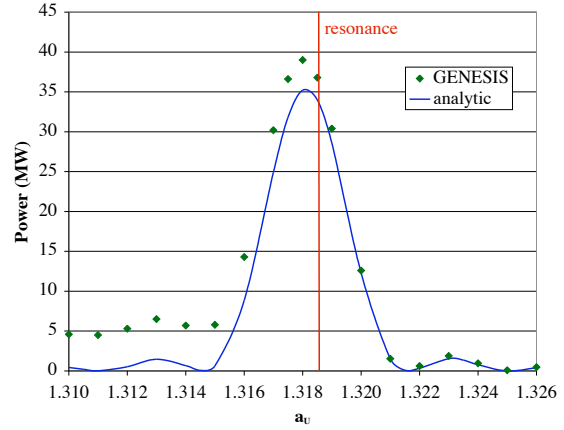


Figure 2: Comparison of analytic theory with simulations using GENESIS. Results for harmonic generation at 1.04 nm, as dipole field strength (a_u) is varied.

the form of higher-order transverse modes, with values of $M^2 \sim 10$. This radiation is generated by particles having large transverse amplitude, which also move forward more slowly. When the magnetic field is too high these higher-order modes do not appear, because there are no particles moving fast enough to be in resonance. For earlier stages which are not emittance-limited, the analytic calculations are in much closer agreement with numerical simulations.

Other sources of error are the nonlinearity of the interaction, where the FEL instability or trapping may increase the output power; the neglect of betatron motion and betatron phase mixing, which may decrease the output power; and an oversimplification of the geometry of each stage of harmonic generation. In the above examples, the FEL instability is unimportant. For example, in the 1.04 nm case, simulations at low beam current, when the FEL gain length is much longer than the total length of the system, would scale to a total output power of 38.9 MW at 500 A. However, for larger values of the applied energy modulation, nonlinear effects become important for reducing particle slippage and maintaining a large bunching parameter.

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